

CLAIMS

WE CLAIM:

1. A method of segmentally modeling real and imaginary parts of dielectric functions with Kramers-Kronig (K-K) consistency, comprising the steps of:

a) providing an imaginary part of a dielectric function over spectroscopic range, and dividing said spectroscopic range into a plurality of segments;

b) fitting each said segment in said spectroscopic range with an approximating K-K consistent oscillator structure, said approximating oscillator structure in each said segment beginning and ending at the start and end of said respective segment, such that a summation of contributions from said oscillator structures present at each point within said spectroscopic range approximates said imaginary part of said dielectric function, and via Kramers-Kronig (K-K) consistency, also the real part of said dielectric function.

2. A method as in Claim 1, in which the segments are of equal spectroscopic range lengths and at least one of said K-K consistent oscillator structures is triangular shaped; the start and end of all oscillator structures, except the start of the first and end of the last, being positioned at the same spectroscopic point as are peaks of immediately adjacent oscillator structures.

3. A method as in Claim 1, in which at least one segment in said spectroscopic range is of a different length than other

segments in said spectroscopic range and at least one of said K-K consistent oscillator structures is triangular shaped; the start and end of all oscillator structures, except the start of the first and end of the last, being positioned at the same spectroscopic points as are peaks of immediately adjacent oscillator structures.

4. A method of segmentally modeling real and imaginary parts of dielectric functions with Kramers-Kronig (K-K) consistent oscillators, comprising the steps of:

practicing steps a and b in either order;

a) providing experimentally obtained data for real and imaginary parts of a dielectric function vs. wavelength for a sample comprising a transparent thin film on a substrate, over a determined range of wavelengths;

b) providing a mathematical model of said sample which comprises a parameter corresponding to the thickness of the transparent thin film and comprises parameters corresponding to a pole amplitude and location at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, then by a global fitting procedure evaluating parameters, including the thickness of the transparent thin film and the location and amplitude of the pole in said mathematical model, utilizing the data corresponding to the real part of the dielectric function;

with transparent thin film thickness evaluated in step b, proceeding to practice steps c, d and e sequentially:

c) defining a wavelength range segment length such that the sum of $(n + 0.5)$ wavelength range segments exactly span the

determined wavelength range, and beginning at one end of said determined wavelength range placing a (K-K) consistent oscillator which comprises an amplitude parameter and begins and ends at the extents of the first segment with its peak midway therebetween, then performing a point by point fit to the imaginary part of the dielectric function data over wavelengths in said first wavelength range segment such that (K-K) consistent oscillator defining parameters are evaluated;

d) placing a second (K-K) consistent oscillator which begins at a wavelength at which the first (K-K) consistent oscillator peaks and ends one wavelength range segment length therefrom and has a peak midway therebetween, then performing a point by point fit to the imaginary part of the dielectric function data over said first and second wavelength range segments such that (K-K) consistent oscillator defining parameters in said first (K-K) consistent oscillator are re-evaluated and oscillator defining parameters in said second (K-K) consistent oscillator are evaluated;

for each of the remaining $(n - 2)$ wavelength range segments, sequentially;

e) placing a (K-K) consistent oscillator which begins at a wavelength at which the just prior (K-K) consistent oscillator peaks and ends one wavelength range segment length therefrom and having a peak midway therebetween, then performing a point by point fit to the imaginary part of the dielectric function data over said wavelength range segments which are fitted with (K-K) consistent oscillators, such that oscillator defining parameters in previously evaluated (K-K) consistent oscillators are re-evaluated and oscillator defining parameters in the added oscillator are evaluated;

such that at each wavelength over the determined range of wavelengths the sum of the contributions of each evaluated (K-K) consistent oscillator approximates the magnitude of the imaginary part of the dielectric function.

5. A method as in Claim 4, in which the pole location and its amplitude at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, are fixed during steps c, d and e.

6. A method as in Claim 4, in which both the data real and imaginary parts the dielectric function data are fitted, and the pole location and/or its amplitude are re-evaluated along with previously evaluated oscillator defining parameters in previously evaluated (K-K) consistent oscillators during steps c, d and e, but wherein said pole location is required to remain located at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths.

7. A method as in Claim 4, in which at least one (K-K) consistent oscillator is of triangular shape.

8. A method as in Claim 4, in which at least one (K-K) consistent oscillator is constructed from at least one polynomial on at least one side of the peak value thereof.

9. A method as in Claim 4, in which at least one (K-K) consistent oscillator is of a shape selected from the group consisting of:

Gaussian;
Lorentzian;
Harmonic;
Ionic1;
Ionic2; and

TOLO.

10. A method as in Claim 4, which further comprises step f:

f) using starting values of parameters previously evaluated performing a global fitting procedure onto both real and imaginary parts of the dielectric function to re-evaluate parameters, including the thickness of the transparent thin film, the location and amplitude of the pole in said mathematical model, and the "N" (K-K) consistent oscillator defining parameters utilizing the data corresponding to the real and imaginary parts of the dielectric function, with a constraining limitation that said pole location is required to remain located at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths.

11. A method as in Claim 10 in which, for each of the "n" the wavelength range segments, the segment length thereof is allowed to float and be fit along with other (K-K) consistent oscillator parameters, with required constraints being:

that the sum of all the resulting $(n + 1/2)$ segment lengths remains equal to the length of the determined wavelength range, and

that for the (2nd - nth) (K-K) consistent oscillator each successive (K-K) consistent oscillator begins at a wavelength at which the just prior $(n - 1)$ (K-K) consistent oscillator peaks.

12. A method as in Claim 4, in which the global and point by point fits are based on a square error minimization criteria.

13. A method as in Claim 9, in which the global and point by

point fits are based on a square error minimization criteria.

14. A method as in Claim 12, in which the global and point by point fits are based on a square error minimization criteria.

15. A method of segmentally modeling real and imaginary parts of dielectric functions with Kramers-Kronig (K-K) consistent oscillators, comprising the steps of:

practicing steps a and b in either order;

a) providing experimentally obtained data for real and imaginary parts of a dielectric function vs. wavelength for a sample comprising a transparent thin film on a substrate, over a determined range of wavelengths;

b) providing a mathematical model of said sample which comprises a parameter corresponding to the thickness of the transparent thin film and comprises parameters corresponding to a pole amplitude and location at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, then by a global fitting procedure evaluating parameters, including the thickness of the transparent thin film and the location and amplitude of the pole in said mathematical model, utilizing the data corresponding to the real part of the dielectric function;

with transparent thin film thickness evaluated in step b, proceeding to practice steps c, d and e sequentially:

c) defining n wavelength range segment lengths such that the sum of said n wavelength range segments plus half the length of the last wavelength range segment at one end of said wavelength range exactly spans the determined wavelength range, and

beginning at the opposite end of said determined wavelength range placing a (K-K) consistent oscillator which comprises an amplitude parameter and begins and ends at the extents of the first segment with its peak midway therebetween, then performing a point by point fit to the imaginary part of the dielectric function data over wavelengths in said first wavelength range segment such that (K-K) consistent oscillator defining parameters are evaluated;

d) placing a second (K-K) consistent oscillator which begins at a wavelength at which the first (K-K) consistent oscillator peaks and ends the second wavelength range segment length therefrom and has a peak midway therebetween, then performing a point by point fit to the imaginary part of the dielectric function data over said first and second wavelength range segments such that (K-K) consistent oscillator defining parameters in said first (K-K) consistent oscillator are re-evaluated and oscillator defining parameters in said second (K-K) consistent oscillator are evaluated;

for each of the remaining $(n - 2)$ wavelength range segments, sequentially;

e) placing a (K-K) consistent oscillator which begins at a wavelength at which the just prior (K-K) consistent oscillator peaks and ends at the n th wavelength range segment length therefrom and having a peak midway therebetween, then performing a point by point fit to the imaginary part of the dielectric function data over said wavelength range segments which are fitted with (K-K) consistent oscillators, such that oscillator defining parameters in previously evaluated (K-K) consistent oscillators are re-evaluated and oscillator defining parameters in the added oscillator are evaluated;

such that at each wavelength over the determined range of wavelengths the sum of the contributions of each evaluated (K-K) consistent oscillator approximates the magnitude of the imaginary part of the dielectric function.

16. A method as in Claim 15 in which the pole location and its amplitude at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, are fixed during steps c, d and e.

17. A method as in Claim 15, in which both the data real and imaginary parts the dielectric function data are fitted, and the pole location and/or its amplitude are re-evaluated along with previously evaluated oscillator defining parameters in previously evaluated (K-K) consistent oscillators during steps c, d and e, but wherein said pole location is required to remain located at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths.

18. A method as in Claim 15, in which at least one (K-K) consistent oscillator is of triangular shape.

19. A method as in Claim 15, in which at least one (K-K) consistent oscillator is constructed from at least one polynomial on at least one side of the peak value thereof.

20. A method as in Claim 15, in which at least one (K-K) consistent oscillator is of a shape selected from the group consisting of:

Gaussian;
Lorentzian;
Harmonic;
Ionic;

Ionic2; and
TOL0.

21. A method as in Claim 15 which further comprises step f:

f) using starting values of parameters previously evaluated performing a global fitting procedure onto both real and imaginary parts of the dielectric function to re-evaluate parameters, including the thickness of the transparent thin film, the location and amplitude of the pole in said mathematical model, and the "N" (K-K) consistent oscillator defining parameters utilizing the data corresponding to the real and imaginary parts of the dielectric function, with a constraining limitation that said pole location is required to remain located at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths.

22. A method as in Claim 19 in which, for each of the "n" the wavelength range segments, the segment length thereof is allowed to float and be fit along with other (K-K) consistent oscillator parameters, with required constraints being:

that the sum of all the resulting segment lengths plus half the last one remain equal to the length of the determined wavelength range, and

that for the (2nd - nth) (K-K) consistent oscillator each successive (K-K) consistent oscillator begins at a wavelength at which the just prior (n - 1) (K-K) consistent oscillator peaks.

23. A method as in Claim 15, in which the global and point by point fits are based on a square error minimization criteria.

24. A method as in Claim 21, in which the global and point by point fits are based on a square error minimization criteria.

25. A method as in Claim 22 in which the global and point by point fits are based on a square error minimization criteria.

26. A method of segmentally modeling real and imaginary parts of dielectric functions with Kramers-Kronig (K-K) consistent oscillators, comprising the steps of:

practicing steps a and b in either order;

a) providing experimentally obtained data for real and imaginary parts of a dielectric function vs. wavelength for a sample comprising a transparent thin film on a substrate, over a determined range of wavelengths;

b) providing a mathematical model of said sample which comprises a parameter corresponding to the thickness of the transparent thin film and comprises parameters corresponding to a pole amplitude and location at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, then by a fitting procedure evaluating parameters, including the thickness of the transparent thin film and the location and amplitude of the pole in said mathematical model, utilizing the data corresponding to the real part of the dielectric function;

with transparent thin film thickness evaluated in step b, proceeding to practice steps c, d and e sequentially:

c) defining a wavelength range segment length such that the

sum of (n) wavelength range segments exactly span the determined wavelength range, and beginning centrally in said determined wavelength range placing a first (K-K) consistent oscillator which comprises an amplitude parameter and begins and ends at the extents of the first segment with its peak midway therebetween;

for each of the remaining (n - 1) wavelength range segments, on either side of the central peak of the first (K-K) consistent oscillator;

d) placing a (K-K) consistent oscillator which begins at a wavelength at which the just centrally prior (K-K) consistent oscillator peaks and ends one wavelength range segment length therefrom and having a peak midway therebetween;

e) performing a fit to the imaginary part of the dielectric function data over said wavelength range segments which are fitted with (K-K) consistent oscillators, such that oscillator defining parameters in the (K-K) consistent oscillators are evaluated;

such that at each wavelength over the determined range of wavelengths the sum of the contributions of each evaluated (K-K) consistent oscillator approximates the magnitude of the imaginary part of the dielectric function.

27. A method as in Claim 26 in which the pole location and its amplitude at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, are fixed during step e.

28. A method as in Claim 26, in which both the real and imaginary parts the dielectric function data are fitted, and the pole location and/or its amplitude are re-evaluated along with

previously evaluated oscillator defining parameters in the (K-K) consistent oscillators during step e, but wherein said pole location is required to remain located at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths.

29. A method as in Claim 26, in which at least one (K-K) consistent oscillators is of triangular shape.

30. A method as in Claim 26, in which at least one (K-K) consistent oscillator is constructed from at least one polynomial on at least one side of the peak value thereof.

31. A method as in Claim 26, in which at least one (K-K) consistent oscillator is of a shape selected from the group consisting of:

Gaussian;
Lorentzian;
Harmonic;
Ionic1;
Ionic2; and
TOLO.

32. A method of segmentally modeling real and imaginary parts of dielectric functions with Kramers-Kronig (K-K) consistent oscillators, comprising the steps of:

practicing steps a and b in either order;

a) providing experimentally obtained data for real and imaginary parts of a dielectric function vs. wavelength for a sample comprising a transparent thin film on a substrate, over a determined range of wavelengths;

b) providing a mathematical model of said sample which comprises a parameter corresponding to the thickness of the transparent thin film and comprises parameters corresponding to a pole amplitude and location at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, then by a fitting procedure evaluating parameters, including the thickness of the transparent thin film and the location and amplitude of the pole in said mathematical model, utilizing the data corresponding to the real part of the dielectric function;

with transparent thin film thickness evaluated in step b, proceeding to practice steps c, d and e sequentially:

c) defining (n) wavelength range segment lengths such that the sum of said (n) wavelength range segments exactly span the determined wavelength range, and beginning centrally in said determined wavelength range placing a first (K-K) consistent oscillator which comprises an amplitude parameter and begins and ends at the extents of the first segment with its peak midway therebetween;

for each of the remaining (n - 1) wavelength range segments, on either side of the central peak of the first (K-K) consistent oscillator;

d) placing a (K-K) consistent oscillator which begins at a wavelength at which the just centrally prior (K-K) consistent oscillator peaks and ends one wavelength range segment length therefrom and having a peak midway therebetween;

e) performing a fit to the imaginary part of the dielectric function data over said wavelength range segments which are

fitted with (K-K) consistent oscillators, such that oscillator defining parameters in the (K-K) consistent oscillators are evaluated;

such that at each wavelength over the determined range of wavelengths the sum of the contributions of each evaluated (K-K) consistent oscillator approximates the magnitude of the imaginary part of the dielectric function.

33. A method as in Claim 32 in which the pole location and its amplitude at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths, are fixed during step e.

34. A method as in Claim 32, in which both the real and imaginary parts the dielectric function data are fitted, and the pole location and/or its amplitude are re-evaluated along with previously evaluated oscillator defining parameters in the (K-K) consistent oscillators during step e, but wherein said pole location is required to remain located at a wavelength beyond the lower wavelength, high energy, extent of said determined range of wavelengths.

35. A method as in Claim 32, in which at least one (K-K) consistent oscillators is of triangular shape.

36. A method as in Claim 32, in which at least one (K-K) consistent oscillator is constructed from at least one polynomial on at least one side of the peak value thereof.

37. A method as in Claim 32, in which at least one (K-K) consistent oscillator is of a shape selected from the group consisting of:

Gaussian;
Lorentzian;
Harmonic;
Ionic1;
Ionic2; and
TOLO.

38. A method as in Claim 26, in which the fits are based on a square error minimization criteria.

39. A method as in Claim 32, in which the fits are based on a square error minimization criteria.

40. A method as in Claim 26, in which ($n = 1$) and the enabling criteria for practicing step d is not met.

41. A method as in Claim 32, in which ($n = 1$) and the enabling criteria for practicing step d is not met.